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13. ABSTRACT (Maximum 200 words)

This report results from a contract tasking A.A.Baikov Institute of Metallurgy, Russian Academy of Sciences as follows: Presentation of report "Principles of the Computer Design of New Inorganic Compounds" at Wright Patterson Laboratory on 27 Nov - 1 Dec 1994.

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Final Report
about Visit to Wright Laboratory and Fall MRS Meeting in Boston

On 27th November-1st December I had met with reseachers of Wright Laboratory (OH). The aims of my visit were a discussions of problems connected with implementation of SPC-94-4097, partaking in Fall MRS Meeting with report and in discussions on prediction of inorganic compounds.

During my visit I presented my report "Principles of the computer design of new inorganic compounds" (Appendix). I discussed with researches from Wright Lab. the principles of the work of programms of the concept formations and problems of their apply to predictions of new inorganic compounds with predefined properties and choice of the best technology for synthesis them. We selected the classes of compounds for prediction according to SPC-94-4097.

The programme of the collaboration in the area of computer design of the new inorganic compounds and development of software for US AF were discussed.

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APPENDIX
PRINCIPLES OF THE COMPUTER DESIGN OF NEW INORGANIC COMPOUNDS

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The problem of the computer-aided design of new materials has two aspects [1-3]. The first aspect is the prediction of compounds, not yet synthesized, which would have predefined properties, using information of the databases, and the choice of the best technology for synthesis them. The second aspect is the search for optimum conditions for the production and for the treatment of the new materials with the aim of optimization of the desired properties. In most cases these two problems can be successfully solved by applying the cybernetic-statistical approach that we suggested [4]. The principal idea of this approach is the combination of the databases on materials and the cybernetic prediction methods used to solve the first problem and the statistical methods of design of the required experiments (or other methods of optimizing) that provide the solution for the second problem.

A.A.Baikov Institute of Metallurgy is now making an information--predicting computer system for the practical realization of this approach [1-3]. This system is intended for the data retrieval on the known compounds, the prediction of inorganic compounds, not yet synthesized, and the forecasting of their properties. This system is based on cybernetic predicting subsystem. Apart from the latter this

information-predicting system employs the database of inorganic compounds, properties, database on elements properties, knowledge base, inferential processor and monitor (see Figure 1). The system is developed for the IBM PC computer.

? Predicting subsystem.

To discuss, in brief, the predicting subsystem, it must be pointed out that a cybernetic approach, developed by us, is based on machine learning strategies.

The chemical foundations of the cybernetic prediction of inorganic compounds are based on Mendelyev's law which asserts that the periodic nature of changes in the properties of chemical systems depends on the nature and properties of the elements which make these systems. The problem of predicting the new compounds was reduced to the analysis of the multidimensional array of property values and the column vector of the desired property. Each row corresponds to some known physico-chemical system, whose class is indicated by row position of column vector. The process of analysing all this information, aimed at finding the classifying regularities, with the help of special programs is referred to as machine learning. By substituting the values of the properties of the components of the unknown system in the regularity thus found, it is possible to determine the class. The implementation of this stage, called the prediction, requires only the knowledge of the values of the component properties.

After testing many programs intended for machine learning applications we fixed on the class of algorithms in which all classifying regularities could be presented in the form of a boolean expression.

The implementation of these machine learning logical algorithms directly involves decreasing the number of searches in the process of formation of the classifying regularities. The algorithm of the inductive concept formation, developed by Prof.Gladun and Dr.Vaschenko [5-8] which we have used for nearly twenty years, solves this particular problem by structuring the computer memory in the form of semantic growing pyramidal networks. The construction of such a network during the input of the objects is followed by learning it, i.e. by singling-out the control vertices determining the class to which the objects belong. The resultant classifying regularities can be stored in computer memory in the form of a learned semantic network or an equivalent Boolean expression in which the meanings of the component properties make the variables. During the prediction process the computer receives only the atomic numbers of the elements or designations of simple compounds, while the values of the properties of the appropriate elements or simple compounds are automatically extracted from the database. After their sampling by means of a special program they are substituted in the classifying regularity and the researcher can easily obtain the necessary prediction.

An important problem of any computer classification is the choice of the properties for the description of physico-chemical systems. This procedure can hardly be formalized completely, but the machine learning algorithm we use [5-8] automatically rejects those properties which have no importance for the classification process. The initial set of the properties for the computer-aided analysis is prepared by the materials scientist and it is desirable that the system of artificial intelligence extrapolates information from this representative set of characteristics.

What properties of the components do we use for the description [1-3, 9-22] ? In the first place, the fundamental properties of chemical elements: distribution of electrons over the energy shells of isolated atoms, ionization potentials, ionic, covalent or atomic radii, melting points, standard entropies of individual substances and the like. In the second place, the properties of simple compounds - oxides, chalcogenides, halides, etc. - are included as required by the composition of the compounds to be predicted.

Using these concepts we have successfully solved the following problems [1-3, 9-22]:

- prediction of compound formation or non-formation for ternary

systems;
- prediction of the formation of the ternary and more complicated systems of desired composition;
- prediction of phases with definite crystal structure types;
- estimation of phase quantitative properties (critical temperature of transition to superconducting state, homogeneity region etc.).

By applying the cybernetic approach we have predicted the formation of thousands of new compounds in ternary, quaternary [1-3, 9-22] and more complicated systems. These compounds were then searched for new semiconductors, superconductors, ferroelectrics, magnets and other materials required for new technologies. The comparison of these predictions with the experimental data, obtained later, showed (see Table) that the average reliability of predicted phases equals about 85 percent. Such a high accuracy for a priori predictions is not ensured by any other known theoretical method.

The best criterion of correctness for any theoretical method is the experimental validation of the prediction. The experimental validation of our theoretical results has shown that this method of cybernetic prediction is an useful tool for the materials scientists and chemists concerned with the a priori prediction of inorganic substances which would have predefined properties.

We return to the information-predicting system [1-3].

? The database of ternary?. ? inorganic compound properties?. is developed by IMET during more then 10 years [23]. At present this database contains information on about 36 000 ternary compounds taken from more then 9 000 publications. The database contains the following information about the ternary systems and compounds (Figure 2). Some of data have been assessed by experts. This database is a part of integrated DB of the inorganic compound properties being developed by IMET.

? The knowledge base?. will store the multidimensional regularities already obtained for various classes of inorganic compounds for their use in the prediction of phases and forecasting of the phase properties. The knowledge will be represented in the form of semantic networks or of their equivalent conjunctive-disjunctive logical expressions.

? Conversational processor?. will manage the conversation of the user with the information-predicting system, as well as giving expert function support in the given application domain.

? The monitor?. will control the computation process and provide the interface between the functional subsystems. In addition, the monitor signals if new experimental data contradict the available regularities. Such contradiction will be eliminated by including new data in the "learning step" and modifying the regularity in the knowledge base.

The information-predicting system is a modified version of expert systems. It differs from conventional expert systems [24-26] in that it employs an unusual procedure of receiving the knowledge from the experts and its subsystem of explanations is of rudimentary nature. From our experience we find that any attempt to make a chemist offer an adequate explanation of the causes of the formation of one phase or another, or the nature of some properties of a compound, usually ends in failure. Instead, the chemist prefers to estimate the autenticity of data concerning the existence of the given compound or the values of the particular phase properties. Therefore we abandoned the idea of making the chemist outline the rules of the formation of inorganic substances with desired properties and decided to make use only of the chemist's expert estimation of the data intended for machine learning. For this reason the explanations subsystem of the information-predicting system is response to the user's inquiry about the nature of one prediction or another can only specify the range of the changes in the properties of the components that determine the phase parental class and indicate the analogs of the predicted compound among the learning examples.

search for optimum conditions for the production of, for the treatment of the new materials.

Considering the prediction of new compound with desired property it is natural to begin the synthesis of this compound. In this case, the problem can be formulated thus: to search the optimal technological conditions which ensure an extremum of the desired property. Some of the mathematical optimizing method can be used for the solution of this problem. For example we succeeded in finding the optimum conditions for the synthesis of Chevrel phase with composition $Ag_x Mo_6 S_6$ and maximum of the critical temperature of transition to superconducting state predicted by us. In this case we have used the statistical methods of the design of the the multifactor experiments. Now my young colleagues N.Kravchenko and V.Petukhov develop the program system for the search for the optimum sections of the acousto-, electro- and nonlinear-optical single crystals using the method by Lagrange and information of our DB on properties of these substances (Figure 3) [27,28].

In that way we have considered a sequential procedure of the design of new compounds with the predefined properties, namely, a database ---> a cybernetic predicting system ---> an optimization of the technology of synthesis or treatment of predicted compounds. The prediction of phases, the forecasting of the desired property, using the information from the database, and the prediction of the best type of technology for synthesis or treatment can be considered as a strategy of the search of substances with the predefined properties. The intrinsic properties of the chemical elements and of the simple compounds are used for description of multicomponent physical-chemical systems on this stage. The known experimental data about substances and about the types of technology for their synthesis are analyzed using computer. The design of experiments or other methods of optimizing for the search for optimal conditions of synthesis or treatment of certain substances, predicted on the first stage, can be considered as the tactics of the search for the new materials. The researcher operates with the technological parameters on this stage.

We considered an automation of the search of the substances on the base of the new information technologies. The researcher can be delivered from the routine work and becomes a creator using his experience and his knowledge as much as possible. Besides intellectualization of the scientific work, this approach allows to promote the search for new substances with predefined properties.

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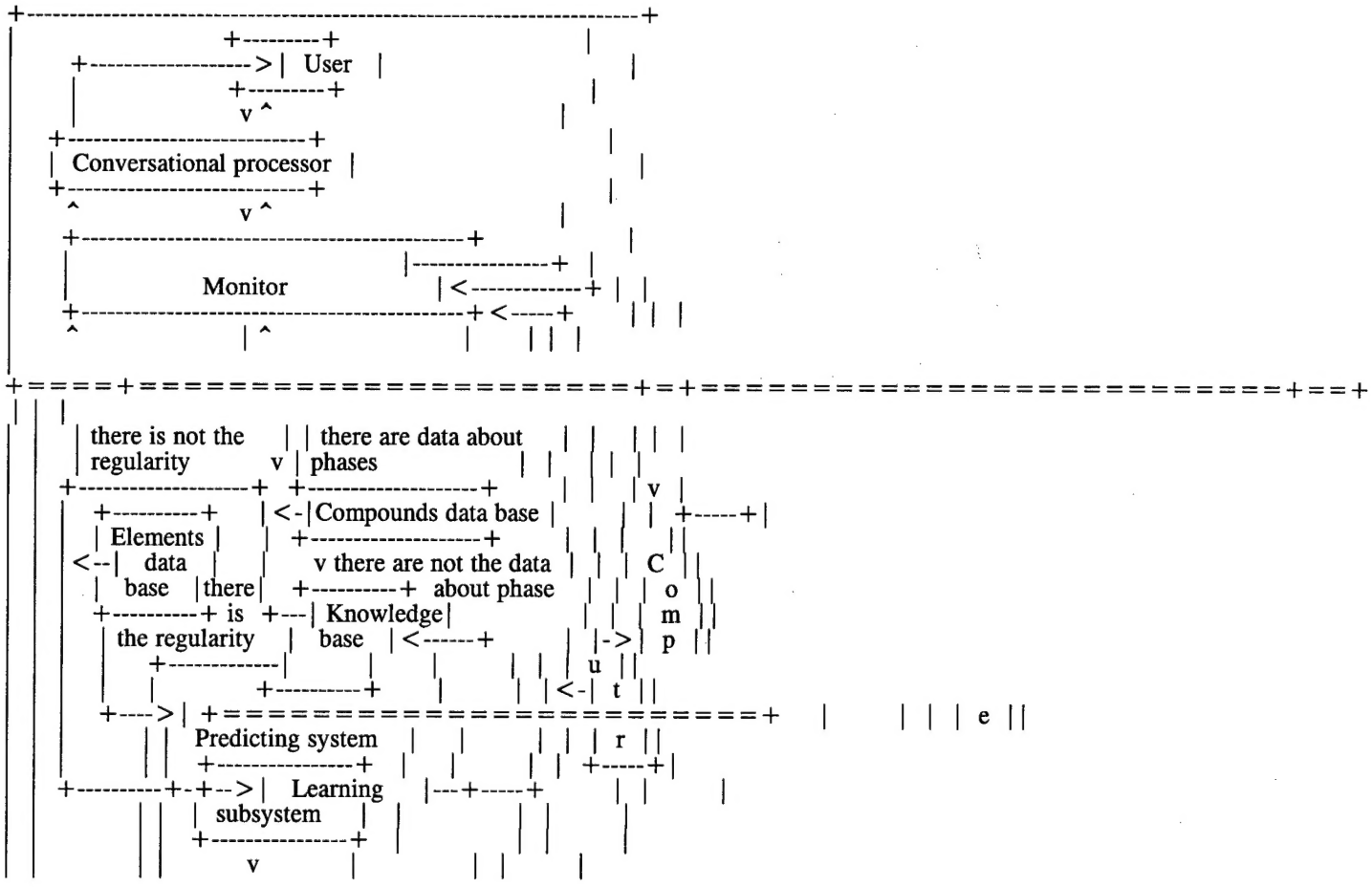
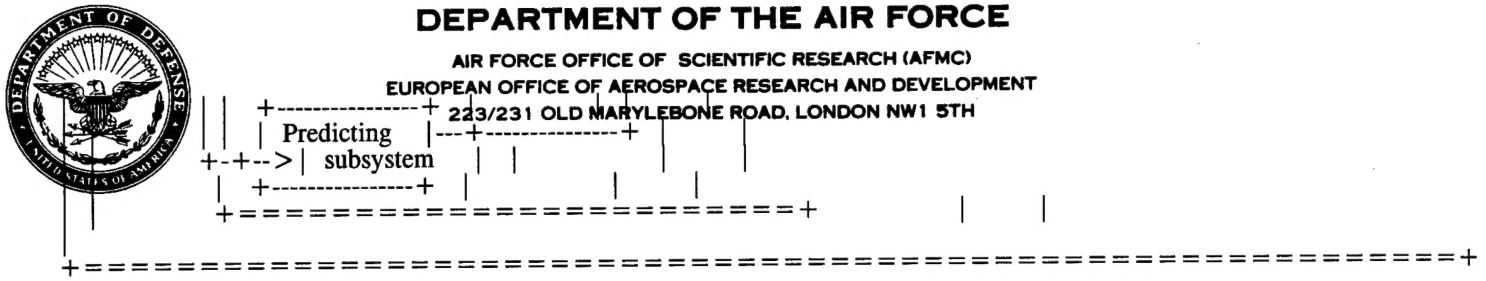
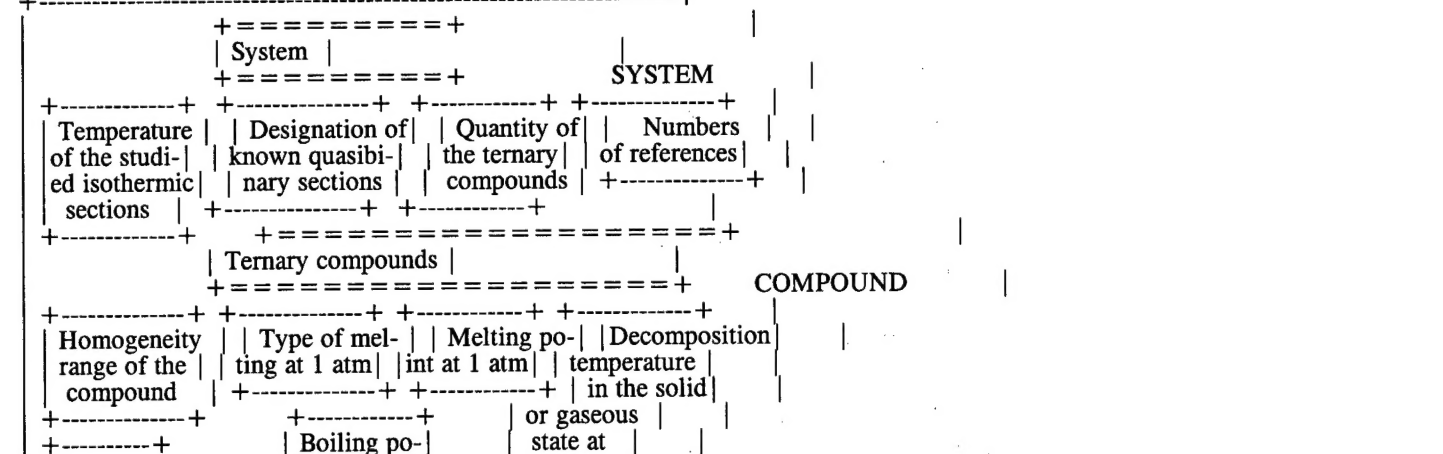




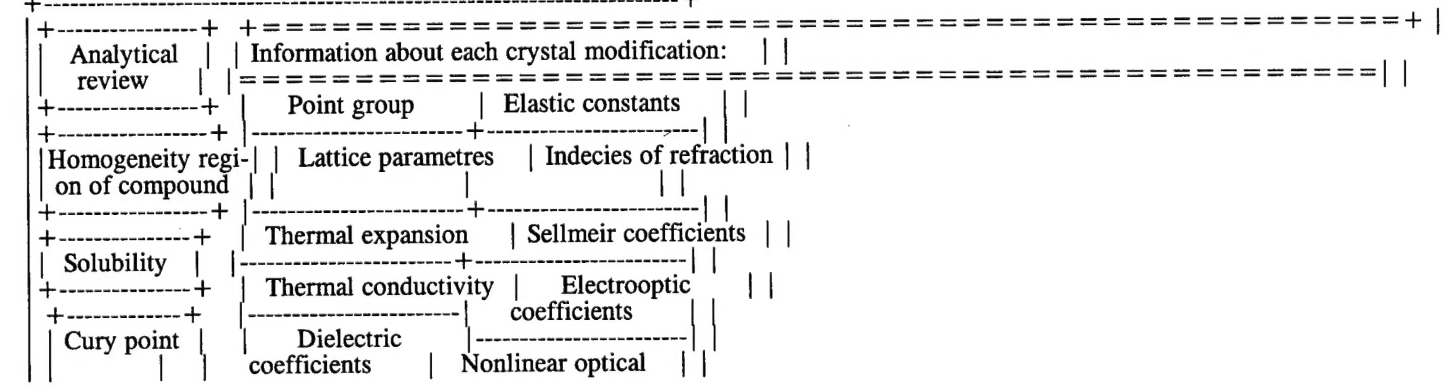
Structure of the information-predicting system

Figure 1



The Database of Ternary Inorganic Compounds "Phases"

Figure 2



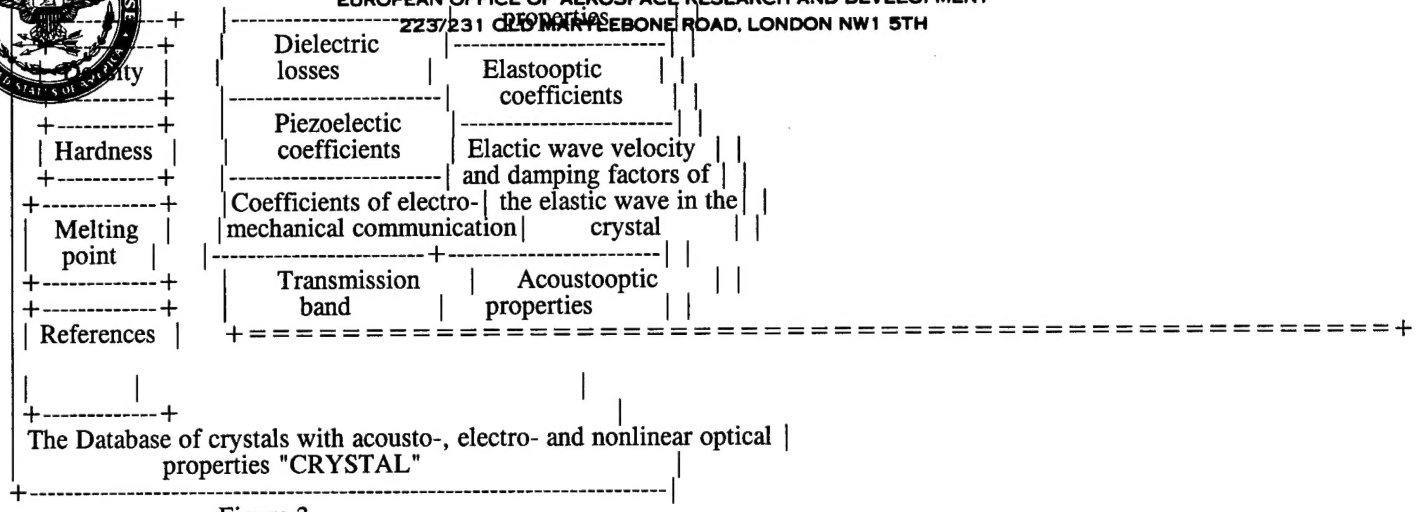


Figure 3

Table
Characteristics of the prediction results for the inorganic phases

Compounds/ systems	Characteristics to be predicted	Number of experimental tests for November,94	Error of prediction, %
ABX (X=Se,Te)	Possibility of formation of compounds	84	45
ABX (X=O,S, Se,Te)	Possibility of formation of compounds	269	11
ABX (X=O,F,S, Cl,Se,Br,Te,I)	Possibility of formation of compounds	351	13
ABX (X=O,F, Cl,Br,I)	Possibility of formation of compounds	332	5
A BX (X=S,Se)	Possibility of formation of compounds	22	9
AB X (X=O,F,S, Cl,Se,Br,Te,I)	Possibility of formation of compounds	480	11
.a w o	Possibility of formation of compounds	83	23
A(Hal) - B(Hal) (Hal=F,Cl,Br,I)	Systems with compounds	94	7
AB X (X=O,S,Se)	Spinel structure type	271	6
.awo	Perovskite structure type	115	23

. | Pyrochlore structure type	69	12	
AB X (X=Al,Si, P,Ge,As,Sb) | ThCr Si structure type	134	7	
ABX (X=Co,Ni, Cu,Pd) | MnCu Al structure type	27	15	
AB X (X=Al,Ga, In) | MnCu Al structure type	24	13	
A (SO)*B (SO) | Possibility of formation of compounds 1:1	81	6	

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